Erroneous solution of three-dimensional (3D) simple orthorhombic Ising lattices

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Alternative abstract

This paper is an invited comment on arXiv:1110.5527 presented at Hypercomplex Seminar 2012 and on sixteen earlier published papers by Zhidong Zhang and Norman H. March. All these works derive from an erroneous solution of the three-dimensional Ising model published in 2007. A self-contained detailed rigorous proof is presented that the final expressions in this work are wrong and that the conjectures on which they are based consequently fail. Further errors and shortcomings in the follow-up works are also pointed out.

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Summary

Thirteen follow-up papers by Zhang and March perpetuate the errors of a 2007 paper by Zhang, which was based on an incorrect application of the Jordan–Wigner transformation and presents final expressions that contradict rigorously established exact results. The presentation given here can be used as a brief mathematical introduction to the Ising model for nonexperts.

1. Introduction

In a very long paper [1] published in 2007 Z.-D. Zhang claims to present the exact solution of the free energy per site and of the spontaneous magnetization of the three-dimensional Ising model in the thermodynamic limit. This claim has been shown to be false [2–7] and we shall show here that very little original work, if any, in [1] can be salvaged.

The principal reason why the outcomes of [1] are wrong is that they contradict exactly known series expansion results [2, 5]. Several references were cited in [2, 5] which show that [1] violates rigorously established theorems. As these cited theorems are formulated for very general lattice models with rather general interactions, requiring complicated notations and such concepts as Banach spaces and Banach algebras, it takes some effort to check that every needed detail is there to make the proof rigorous.

Therefore, we present here a simpler self-contained presentation, restricted to the three-dimensional Ising model on a simple cubic lattice, which can be used as a short introduction for nonexperts interested in this model.

Definition 1.1. The isotropic Ising model on $\mathbb{Z}_n^3$, a periodic $n \times n \times n$ lattice with $N = n^3$ sites $i = (i_x, i_y, i_z)$ on a 3-torus, is defined by its configuration space

$$\mathbb{T}^3 \supset \mathbb{Z}_n^3 \to \{\pm 1\}^N, \qquad i \mapsto \sigma_i = \pm 1, \text{ for } i \in \mathbb{Z}_n^3, \tag{1}$$

and its interaction energy

$$\mathcal{H}_N : \mathbb{Z}_n^3 \to \mathbb{C}, \qquad \mathcal{H}_N = \mathcal{H}_N(\{\sigma_i\}) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - B \sum_i \sigma_i, \tag{2}$$

where the sum over $\langle i,j \rangle$ is over all nearest-neighbor pairs of sites i and j, J is the interaction strength and B is the scaled magnetic field. Sites i and j are nearest-neighbor (nn) sites, if and only if

$$(i_x - j_x, i_y - j_y, i_z - j_z) = (\pm 1, 0, 0),\ (0, \pm 1, 0),\ \text{or } (0, 0, \pm 1) \bmod n. \tag{3}$$

Remark 1.2. The generalization to the orthorhombic lattice is straightforward, replacing n by n, n', n'' and J by J, J', J'' for the three lattice directions. We consider the isotropic lattice for the sake of simplicity of arguments, as this special case suffices to disprove Zhang's claims [1].

Definition 1.3. Given a function $A \equiv A(\{\sigma\})$ of the spin configuration, its expectation value is

$$\langle A\rangle_N = \frac{1}{Z_N}\sum_{\{\sigma_i=\pm 1\}} A\,\mathrm{e}^{-\beta\mathcal{H}_N}, \qquad \langle A\rangle = \lim_{N\to\infty}\langle A\rangle_N, \tag{4}$$

where the partition function,

$$Z_N = \sum_{\{\sigma_i=\pm 1\}} \mathrm{e}^{-\beta\mathcal{H}_N}, \tag{5}$$

is a state sum taken over all 2^N spin configurations, while $\beta = (kT)^{-1}$ with T the absolute temperature and k Boltzmann's constant. If β, J, and B are real, then $\rho(\{\sigma\}) = \mathrm{e}^{-\beta\mathcal{H}_N}/Z_N$ is the Boltzmann-Gibbs canonical probability distribution.

Definition 1.4. The free energy per site f_N and its infinite system limit f are given by

$$-\beta f_N = \frac{1}{N}\log Z_N, \qquad f = \lim_{N\to\infty} f_N, \tag{6}$$

whereas the spontaneous magnetization is defined by

$$I = \lim_{B\downarrow 0}\lim_{N\to\infty}\langle\sigma_{i_0}\rangle_N = \lim_{B\downarrow 0}\lim_{N\to\infty}\frac{1}{Z_N}\sum_{\{\sigma_i=\pm 1\}}\sigma_{i_0}\,\mathrm{e}^{-\beta\mathcal{H}_N}, \tag{7}$$

with i_0 any of the N lattice sites, as the lattice is chosen periodic. The pair-correlation function of spins at sites i and j is $\langle\sigma_i\sigma_j\rangle$,

Remark 1.5. As in [1], we shall concentrate on the zero-field ($B = 0$) thermodynamic limit ($\lim_{N\to\infty}$). The order of limits in (7) was used implicitly in Yang's paper [8] on the spontaneous magnetization of the square-lattice Ising model [9–11]. With the opposite order of limits the result is identically zero. An alternative definition is $I^2 = \lim\langle\sigma_i\sigma_j\rangle|_{B=0}$ in the limit of infinite separation of sites i and j [12].

In [1] Zhang starts out mimicking the treatment of the two-dimensional Ising model by Onsager and Kaufman [9–11], in order to calculate the free energy, magnetization and pair correlation of the three-dimensional case. Even though Zhang made two early errors in [1], while transforming to Clifford algebra operators and treating boundary terms [5], he claims [6] that these are overcome by two conjectures. But these conjectures are based on no serious evidence whatsoever and

the resulting expressions for the free energy and magnetization [1] are demonstrably incorrect, as they fail the series test [2, 5].

First, in section 2, a detailed account will be given of the rigorous results of the 1960s violated by Zhang's work. Theorems 2.8 and 2.9 provide rigorous proof of the correctness of the series test. Then, in section 3, further comments will be presented, including several on the follow-up work by March and Zhang [13–25], which contain several additional errors and misleading statements.

2. Some rigorous results of the 1960s revisited

In recognizing the criticisms to which his work in [1] has been subjected in [2, 4, 5, 7], Zhang (supported more recently by Norman H. March) has argued that the usual high-temperature series expansions [26], renormalization group treatments [27, 28], and Monte Carlo simulations [29, 30], fail to apply in the vicinity of infinite temperature owing to singular behavior and Yang–Lee zeros [31, 32] present even in the thermodynamic limit. Hence, it is argued, such criticisms are not applicable as a basis for criticizing the quite different conclusions he has reached. See specifically the claims Zhang has made in the second paragraph of [3], and in the second half of page 766 of [6], as well in section 5 of [16], second half of page 534. The aim of this section is to show specifically by a detailed mathematical analysis that there is no credibility at all in these claims.

In fact, five decades ago several theorems were published and supported by fully rigorous proofs that underpin the validity of the criticisms of Zhang's work, see, e.g., [33, 34] for review. Nevertheless, let us here take the reader through a simplified treatment especially tailored to apply to the point at issue, namely, the statistical mechanics of the Ising model on a cubic lattice with periodic boundary conditions.

The proof of the thermodynamic (infinite system-size) limit of the free energy typically uses the following lemma, see e.g. (2.15) in [33]:

Lemma 2.1.

$$|\log \mathrm{Tr}\, \mathrm{e}^{A} - \log \mathrm{Tr}\, \mathrm{e}^{B}| \leqslant \|A - B\|, \quad \textit{for } A \textit{ and } B \textit{ hermitian.} \tag{8}$$

Proof. The proof follows immediately working out

$$\log \mathrm{Tr}\, \mathrm{e}^{A} - \log \mathrm{Tr}\, \mathrm{e}^{B} = \int_0^1 \frac{d}{dh} \log \mathrm{Tr}\, \mathrm{e}^{B+h(A-B)} dh = \int_0^1 \frac{\mathrm{Tr}\,(A-B)\mathrm{e}^{B+h(A-B)}}{\mathrm{Tr}\, \mathrm{e}^{B+h(A-B)}} dh,$$

where the last integrand is an expectation value. (In this paper we only need to consider the commuting case that A and B are diagonal matrices.) ∎

Theorem 2.2. *The free energy per site f_N converges uniformly to a limit f as the system size becomes infinite for βJ real and bounded.*

Proof. In order to prove this we must estimate $|f_N - f_M|$ for $N, M > N_0$, with N_0 sufficiently large. Here we do that only for periodic cubic lattices $N = n^3$, $M = m^3$ and compare with the larger periodic cubic lattice of size $NM = (nm)^3$. By changing a subset of the interactions we can change the larger lattice into N identical cubes of the size M lattice, or the other way around. The proof is then provided by counting the changed interactions and by using Lemma 8. In our case, the trace in the lemma is just the sum over spin configurations and the norm the maximum over all configurations. ■

Remark 2.3. Lemma 2.1 can also be used to show that the free energy f does not depend on boundary conditions in the large system limit with different shapes than cubes, provided it is taken in the sense of van Hove, see e.g. [33, 34] for details.

Remark 2.4. The proof of Theorem 2.2 gives a rigorous bound on the difference of the free energy per site of a finite system and its large-system limit. It can therefore be used to estimate the accuracy of finite-size calculations using e.g. Monte Carlo simulations.

Lemma 2.5. *The partition function Z_N (5) is a Laurent polynomial in $\mathrm{e}^{\beta J}$, so that βf_N is singular only for the zeros of this Laurent polynomial and for $\mathrm{e}^{\beta J} = \infty$. As Z_N is a sum of positive terms for real βJ, it cannot have zeros on the real axis.*

We will show that the zero closest to $\beta J = 0$ (or $\mathrm{e}^{\beta J} = 1$) in the complex βJ plane is uniformly bounded away, i.e. $Z_N \neq 0$ for all $|\beta J| < K_0$ and all N for some fixed K_0. This means that f_N can be expanded in a power series in βJ that is absolutely convergent for $|\beta J| < K_0$ and uniform in N. It is well known that more and more coefficients become independent of N as N increases. Together this implies that the limiting f also has a power series in βJ with radius of convergence at least K_0.

We continue by deriving a lower estimate for K_0. Most proofs of the analyticity of free energies and correlation functions use linear correlation identities of Schwinger–Dyson type, known under such names as the BBGKY hierarchy, Mayer–Montroll or Kirkwood–Salzburg equations. We could use [35] and [36]. But instead, let me give an alternative proof using an identity of Suzuki [37, 38], restricted to the isotropic Ising model on a simple cubic lattice with periodic boundary conditions and of arbitrary size, as this method also can be used to generate the coefficients of the high-temperature series. More precisely, using the canonical definition of the expectation value of a function $A \equiv A(\{\sigma\})$ of the spin configuration, we have the correlation identity [37, 38]:

Lemma 2.6. *(M. Suzuki, 1965 [37, 38])*

$$\Big\langle \prod_{i=1}^{m} \sigma_{j_i} \Big\rangle_N = \frac{1}{m} \sum_{k=1}^{m} \Big\langle \Big(\prod_{\substack{i=1 \\ i \neq k}}^{m} \sigma_{j_i} \Big) \operatorname{tgh} \Big(\beta J \sum_{l \text{ nn } j_k} \sigma_l \Big) \Big\rangle_N, \tag{9}$$

where $j_1, \ldots, j_m$ are the labels of m spins and l runs through the labels of the six spins that are nearest neighbors of σ_{j_k}.

Proof. The proof of (9) is easy summing over spin σ_{j_k} in the numerator of the expectation value, i.e.,

$$\sum_{\sigma_{j_k}=\pm 1} \sigma_{j_k} \mathrm{e}^{\beta J \sum_{l \text{ nn } j_k} \sigma_{j_k} \sigma_l} = \operatorname{tgh} \Big(\beta J \sum_{l \text{ nn } j_k} \sigma_l \Big) \sum_{\sigma_{j_k}=\pm 1} \mathrm{e}^{\beta J \sum_{l \text{ nn } j_k} \sigma_{j_k} \sigma_l}. \tag{10}$$

Averaging over k has been added in (9), so that all spins are treated equally, consistent with the periodic boundary conditions. The lemma is also valid without that. ∎

Next we use

Lemma 2.7.

$$\operatorname{tgh} \Big(\beta J \sum_{l=1}^{6} \sigma_l \Big) = a_1 \sum_{(6)} \sigma_l + a_3 \sum_{(20)} \sigma_{l_1} \sigma_{l_2} \sigma_{l_3} + a_5 \sum_{(6)} \sigma_{l_1} \sigma_{l_2} \sigma_{l_3} \sigma_{l_4} \sigma_{l_5}, \tag{11}$$

where the sums are over the 6, 20, or 6 choices of choosing 1, 3, or 5 spins from the given $\sigma_1, \ldots, \sigma_6$. It is easy to check that the coefficients a_i are

$$a_1 = \frac{t(1 + 16t^2 + 46t^4 + 16t^6 + t^8)}{(1 + t^2)(1 + 6t^2 + t^4)(1 + 14t^2 + t^4)}, \qquad a_3 = \frac{-2t^3}{(1 + t^2)(1 + 14t^2 + t^4)},$$

$$a_5 = \frac{16t^5}{(1 + t^2)(1 + 6t^2 + t^4)(1 + 14t^2 + t^4)}, \qquad t \equiv \operatorname{tgh}(\beta J). \tag{12}$$

The poles of the a_i are at $t = \pm \mathrm{i}$, $t = \pm(\sqrt{2} \pm 1)\mathrm{i}$, and $t = \pm(\sqrt{3} \pm 2)\mathrm{i}$. It can also be verified, e.g. expanding the a_i in partial fractions, that the series expansions of the a_i in terms of the odd powers of t alternate in sign and converge absolutely as long as $|\beta J| < \operatorname{arc\,tg}(2 - \sqrt{3}) = \pi/12$.

Proof. Clearly, the tanh in (11) can be expanded as done. Replacing all six spins, σ_l by $-\sigma_l$, shows that no terms with an even number of spins occur. Also, permutation symmetry allows only three different coefficients. Multiplying (11) with one, three, or five spins σ_l and then summing over all $2^6 = 64$ spin states, is one way to derive (12). It is then straightforward to verify the following partial fraction expansions,

$$\begin{aligned} a_{1,5} &= \frac{1}{24} \Big(\frac{p_1 t}{1 + (p_1 t)^2} + \frac{p_2 t}{1 + (p_2 t)^2} \Big) \pm \frac{\sqrt{2}}{8} \Big(\frac{p_3 t}{1 + (p_3 t)^2} + \frac{p_4 t}{1 + (p_4 t)^2} \Big) \\ &\quad + \frac{1}{3} \frac{p_5 t}{1 + (p_5 t)^2}, \\ a_3 &= \frac{1}{24} \Big(\frac{p_1 t}{1 + (p_1 t)^2} + \frac{p_2 t}{1 + (p_2 t)^2} \Big) - \frac{1}{6} \frac{p_5 t}{1 + (p_5 t)^2}, \end{aligned} \tag{13}$$

$$p_{1,2} = 2 \pm \sqrt{3}, \quad p_{3,4} = \sqrt{2} \pm 1, \quad p_5 = 1, \qquad (p_1 p_2 = p_3 p_4 = 1). \tag{14}$$

The remaining statements of the lemma follow from these expansions. ∎

We can now prove the following two theorems for magnetic field $B = 0$:

Theorem 2.8. *The correlation functions $\langle \prod_{i=1}^m \sigma_{j_i} \rangle_N$ and their thermodynamic limits $\langle \prod_{i=1}^m \sigma_{j_i} \rangle$ are analytic, having series expansions in t or βJ with radius of convergence bounded below by (17) and uniformly convergent for all N including $N = \infty$. Let d be the largest edge of the minimal parallelepiped containing all sites $j_1, \ldots, j_m$. Then the coefficient of t^k with $k < n - d$ for the lattice with $N = n^3$ sites equals the corresponding coefficient for larger N, including the one for $N = \infty$.*

Proof. We can assume that $m > 0$ and even, since for m odd we have $\langle \prod_{i=1}^m \sigma_{j_i} \rangle_N \equiv 0$ as it both is invariant and changes sign under the spin inversion $\sigma_i \to -\sigma_i$ for all sites i.

The system of equations (9)–(12) can be viewed as a linear operator on the vector space of linear combinations of all correlation functions of the 3-dimensional Ising model. It is easy to estimate the norm of this operator. Using the alternating sign property of the a_i's, it is easy to verify that a_1, a_3, and a_5 can all be written as t times a series in t^2, which three series consist of positive terms only when t is imaginary. This means that each $|a_i|$ is maximal for given $|t|$ when t is imaginary and within the radius of convergence, i.e. p_2 in (14).

From the $32m$ terms in the right-hand side (RHS) of (9) after applying (11), it follows then that we only need to study

$$6a_1 + 20a_3 + 6a_5 = \frac{2t(t^2+3)(3t^2+1)}{(1+t^2)(1+14t^2+t^4)} \tag{15}$$

for purely imaginary t to find the desired upper bound r for the norm. Setting $t = \mathrm{i}x$ with $0 < x < 2 - \sqrt{3}$ to stay within the first pole of (15), we next define

$$r = \frac{2x(3-x^2)(1-3x^2)}{(1-x^2)(1-14x^2+x^4)}, \qquad \text{for } x = |t|. \tag{16}$$

We then have that the RHS of (9) is bounded by rM, where $M = \max |\langle \sigma \cdots \sigma \rangle|$ with the maximum taken over all $32n$ pair correlations in the RHS. (Obviously, $M \leqslant 1$ if $\beta \geqslant 0$ and real, but we shall not use this.) We can easily show that $r < 1$ for

$$\begin{aligned} &|t| < (\sqrt{3}-\sqrt{2})(\sqrt{2}-1) = 0.131652497\cdots, \quad \text{or} \\ &|\beta J| < \operatorname{arc\,tg}[(\sqrt{3}-\sqrt{2})(\sqrt{2}-1)] = 0.130899693\cdots. \end{aligned} \tag{17}$$

To prove analyticity of $\langle \prod_{i=1}^m \sigma_{j_i} \rangle_N$ as a function of β at $\beta = 0$, we apply (9) to it. Then we apply (9) to each of the $32m$ new correlations, and we keep repeating this process ad infinitum. Since $\sigma_i^2 = 1$, we will from some point on regularly encounter the correlation with $m = 0$, i.e. zero σ factors, for which $\langle 1 \rangle = 1$, so that the iteration process ends there. Each other correlation (with $m > 0$) vanishes with at least one power of t, as can be seen comparing e.g. (9) and (12). We conclude that the iteration

process generates the high-temperature power series in t to higher and higher orders, for arbitrary given size N of the system.

To get the partial sum of the series to a given order, we only need to keep the contributions for which the iteration process has ended and expand all occurring a_i as series in t. The sum of the absolute values of the terms is bounded by $\sum r^j < \infty$ when (17) holds. However, the original correlation function is meromorphic with a finite number of poles away from the real t axis for any finite N. Thus for sufficiently high order of series expansion in t, the remainder term is arbitrarily small. The only possible conclusion is that we have proved convergence of the series expansion of $\langle\prod_{i=1}^m \sigma_{j_i}\rangle_N$ in powers of t, uniform in N with a finite radius of convergence in the complex t and β planes bounded below by (17).

To prove the final statement of the theorem for finite N, we notice that the above iteration process generates new correlations with the range of the positions j of the spins extended by one in a given direction. As long as we do not go around a cycle (periodic boundary condition) of the 3-torus, we do not notice any N-dependence. It takes at least $n-d$ iteration steps to notice the finite size of the lattice.

Combining the convergence uniform in N with the fact that more and more coefficients converge with increasing N, we conclude that $\langle\prod_{i=1}^m \sigma_{j_i}\rangle_N$ converges to a unique limit as $N \to \infty$ for $|t| < 2-\sqrt{3}$, with the properties stated in the theorem. ∎

Theorem 2.9. *The reduced free energy βf_N for arbitrary N and its thermodynamic limit βf are analytic in βJ for sufficiently high temperatures. They have series expansions in t or βJ with radius of convergence bounded below by (17) and uniformly convergent for all N including $N=\infty$. The first $n-1$ coefficients of these series for $N=n^3$ equal their limiting values for $N=\infty$.*

Proof. To prove analyticity of βf in terms of β at $\beta=0$ it suffices to study the internal energy per site or the nearest-neighbor pair correlation function, as

$$u_N = \frac{1}{N}\langle\mathcal{H}_N\rangle_N = \frac{\partial(\beta f_N)}{\partial\beta} = -3J\langle\sigma_{0,0,0}\sigma_{1,0,0}\rangle_N, \tag{18}$$

as follows from (5) and (6). Here $\sigma_{0,0,0}$ and $\sigma_{1,0,0}$ can be any other pair of neighboring spins. The proof then follows from Theorem 2.8 and integrating the series for u_N, using $Z_N|_{\beta=0} = 2^N$, implying $\lim_{\beta\to 0}\beta f_N = -\log 2$. ∎

Remark 2.10. Adding a small magnetic field B and generalizing the steps in the above, we can conclude that all correlation functions are finite for small enough $|\beta|$ and $|\beta H|$, so that there are no Yang–Lee zeros [31, 32] near the $H=0$ axis for small β and H. The proof can also be generalized to the case that the interactions are anisotropic, i.e. J, J', J'' as in [1]. Then Z_N is a Laurent polynomial in each of $\mathrm{e}^{\beta J}$, $\mathrm{e}^{\beta J'}$, and $\mathrm{e}^{\beta J''}$, etc.

Remark 2.11. Similar results can be derived for the low-temperature series, for example after applying the Kramers–Wannier duality transform to the high-temperature regime of the dual system with spins in the centers of the original cubes and with four-spin interactions around all cube faces perpendicular to the edges of the original lattice [39].

Remark 2.12. It is straightforward to calculate the first few high-temperature series coefficients of the free energy by the method described in this section, with or without using the averaging in (9). They agree with the long series reported in [26] and earlier works cited there. Zhang's free energy formula claimed for all finite temperatures [1] does not agree, as already the coefficients of $\kappa^2 \equiv t^2$ in (A12) and (A13) of [1] differ. Zhang's excuse that there are two expansions, one for finite β and one for infinitesimal β, violates general theorems, that apply to more general models than the Ising model [4,5]. Here this excuse is invalidated in detail by Theorem 2.9.

Remark 2.13. Zhang's spontaneous magnetization series is obviously wrong. In three dimensions one should have $I - 1 = \mathrm{O}(x^6)$, with $x \equiv \mathrm{e}^{-\beta J}$ in the low-temperature limit, $x \to 0$ $(J > 0)$, as each spin has six nearest neighbors [5], rather than eight, which would result in the four-dimensional $I - 1 = \mathrm{O}(x^8)$ presented by Zhang in (103) of [1].

Remark 2.14. The finite radius of convergence of the series expansions about $\beta = 0$ is also hinted at by the fact that the zeros of Z_N for $T = \infty$ occur for $B = \pm\mathrm{i}\infty$, $\beta B = \pm\mathrm{i}\pi/2$ [7]. For fixed temperature T or $\beta = 1/kT$ and $\beta J > 0$ real the zeros of Z_N lie on the unit circle in the complex $\mathrm{e}^{-2\beta B}$ plane [32], all located at -1 at infinite temperature [7] and spreading out with decreasing temperature until the zeros "pinch" $+1$ on both sides of the unit circle at and below the critical temperature, in agreement with the theory of Yang and Lee [31,32]. Zhang's claim that this pinching at $+1$ also occurs at $\beta = 0$ [1,3,6,16] is disproved by Theorem 2.9.

Corollary 2.15. *As pointed out already in [2,4,5], all final results of [1] are proven wrong, as they do not agree within a finite radius of convergence with the well-known series expansion coefficients. This also means that the conjectures of [1] are falsified.*

3. Further remarks and objections

3.1. Two series expansions for the same object

In appendix A of [1] Zhang claims to reproduce the first 22 terms of the high-temperature series for the free energy. But this is no more than reverse engineering, fitting the known coefficients [26] to an integral transform (A.1) or (74) in [1] giving the first few coefficients of the weight functions as given in (A.2). There is no more information than the series results provided by others, so that this does not constitute a new result, as explained in [2, 5].

As this construction this way is based on a conjectured integral transform of weight functions that can only be reconstructed from a few known series coefficients, it cannot be considered an exact solution. Knowing this, Zhang conjectures ad hoc above (A.3) on page 5400 another choice for the weight functions, namely $w_x = 1$, $w_y = w_z = 0$, leading to another high-temperature series for non-infinitesimal temperatures, in violation of the rigorous result on the uniqueness of the series expansion presented in section 2. This is not sound mathematics [2].

3.2. Citations by other authors

The outcomes of [1] have been criticized in [29, 30], as they disagree with recent high-precision Monte Carlo calculations presented there. Both the position of the critical point and the values of the critical exponents differ from the ones in [1], while the results of [29, 30] agree with those of many others obtained by a variety of methods [28].

One paper on a decorated three-dimensional Ising model [40], mapping this model exactly to the Ising model on a cubic lattice, used Zhang's free energy [1] as an approximate result in the analysis. The experimental paper [41] states that their result for the critical exponent $\Delta = 2.0 \pm 0.5$ is consistent with [1]. However, the reported error bar is so large that this means nothing. Moreover, paper [42] on the Heisenberg model only briefly cites [1] as an Ising reference.

The authors of [43, 44] learned from [1] the quaternion setup of the transfer matrix of the three-dimensional Ising model, which was well-known earlier, see e.g. [45–47].[1] In Zhang's work [1] this is treated before the first error occurs with the Jordan–Wigner transformation to Clifford algebra operators. His P's and Q's do not anticommute [5, 6].

[1] Maddox only published his final formula for the free energy [45]. The details were discussed in a special session, where also his error (the same as Zhang's first error [5]) was discovered.

3.3. Advertising wrong critical exponents

Klein and March took the exact Ising critical exponents for dimensions $d = 1, 2, 4$ together with the proposal of [1] for $d = 3$ and made an ad hoc fit [48] for all real $1 \leqslant d \leqslant 4$. However, they failed to compare with the results from ε-expansion [27,28], where $\varepsilon = 4 - d$. This is a serious shortcoming, as the [48] formulae disagree with the ε-expansion exponents for small ε and fail the one foremost explicit test available. It may also be noted that the extrapolated Ising exponents for $d = 3$ from ε-expansion agree with those extracted from series expansions and Monte Carlo calculations [28], while differing from those presented in [1].

March and Zhang have followed this paper [48] up with thirteen publications, thus perpetuating the errors of the original work [1]. Some of these works compare Zhang's critical exponents with those from experiments on $CrBr_3$ and Ni [13, 14]. Nickel is known to have Heisenberg exchange interactions and its critical exponent β is about the accepted value for the three-dimensional Heisenberg model, which is also about Zhang's value wrongly claimed for Ising.

Comparing experiments with models needs a discussion of the interactions in the experimental compounds, whether Ising or Heisenberg, isotropic or anisotropic, short-range or long-range, etc. No such analysis was presented. The same objection can be brought up about section 2 of [20].

In [15] critical exponents for the two- and three-dimensional q-state Potts model are discussed. Those for $d = 2$ are by now well established, but the values presented for $d = 3$ cannot all be correct, as for the Ising case $q = 2$ the exponents of [1] have been used.

In [18,19] a new formula for critical exponent δ is given, improving the one in [48]. The same objection still applies, as again no comparison with ε-expansion is made.

It is implied by the theory of Yang and Lee [31, 32], that the best experimental results on Ising exponents are to be expected from measurements on liquid-gas transitions in simple substances. March and Zhang have admitted that the exponents of [1] fail this test, see section 3 of [20]. Their suggestion that the experiment needs to be redone carries no credibility, as the critical exponents measured in a number of similar experiments are indeed typical for Ising, see section 3.2.2 of [28].

3.4. Singularity of free energy at $T = \infty$

Several statements in section 5 of [16] repeat and expand on statements in [1, 3, 6] contradicting rigorous theorems discussed in section 2 above. For example, while it is correct that the free energy f diverges at $T = \infty$, this does not correspond to a physical singularity, as the combination βf is to be used. Indeed, $\mathrm{e}^{-\beta f}$ relates to the normalization of the Gibbs ensemble probability distribution and βf is the principal object of Theorem 2.9. Multiplying βf with kT results in f having a convergent Laurent expansion with a leading pole at $T = \infty$ that has no physical significance. Another point is discussed in Remark 2.14 in section 2.

3.5. False argument for $\alpha = 0$

Paper [17] addresses tricritical behavior. The authors claim that the logarithmic divergence of the specific heat, $\alpha = 0$ (log) at tricritical points in three dimensions, supports the similar value reported in [1] for the Ising critical behavior. However, this reasoning is flawed lacking any theoretical basis and contradicts the accepted value $\alpha = 0.110 \pm 0.001$, see eq. (3.2) and tables 3–7 of [28].

3.6. The $\epsilon = d - 2$ expansion

In papers [21, 22] on Anderson localization the authors say that $\epsilon = d - 2$ is not a small parameter for $d = 3$, just like $\varepsilon = 4 - d$ of the ε-expansion is not. This ignores that the best ε-expansion extrapolation results agree remarkably well with those from series, Monte Carlo, and experiment [28]. This argument to support [1] is again not valid.

3.7. Higher dimensions

The combinatorial sums defining the 3-dimensional Ising model involve commuting spin variables and an interaction energy that is a function of these spins. There is no reason to introduce time and quantum mechanics in this classical system, as is done in [23]. On the other hand, introducing the transfer matrix changes one space coordinate to (discrete) imaginary time. After "Wick rotation" to real time the 3-dimensional Ising model relates to a (2+1)-dimensional quantum system. The fourth dimension introduced in [1] has only been used to obtain wrong results violating rigorous results.

3.8. Fractal dimensions based on wrong results

In [24] Zhang and March write down some proposals for fractal dimensions. However, the values given for dimension 3 are based on incorrect results of [1].

3.9. Unfounded Virasoro algebra

The most recent paper [25] uses the weight factors of [1] to introduce a Virasoro algebra in 3+1 dimensions. This is ad hoc and the notations in equation (5) and seven lines below (6) there are not mathematically sound. To take the real part of the absolute value of a phase factor instead of just writing 1 makes no sense. Also, the Virasoro algebra relates to an infinite dimensional symmetry, which is only consistent with conformal symmetry in two dimensions, see e.g. [49]. Therefore, [25] has fundamental errors.

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Open letter to Dr. Zhang in response to arXiv:1209.3247

After posting arXiv:1209.3247 Dr. Zhang sent me an email ending with "Any further criticisms or comments from you are welcome." The following is a LaTeX version of the body of my September 17 email reply:

First of all, the comment arXiv:1209.0731 contains very little that is in my published earlier Comment and Rejoinder. There is some material from the unpublished additions to the arXiv version of the Rejoinder, but that part is much improved with several new details added. There are also some pages discussing papers published later. Therefore, the statement "hard to find anything new" is wrong. Also, several statements are not even addressed in the Response and cannot be covered with the "unnecessary to repeat all of Zhang's responses".

Conjecture 1 is not backed up by any quantitative evidence in the original 117 page work. The validity can at this moment only be judged by the resulting free energy. In my section 3.1, I make clear that the result becomes an integral transform from the weight functions to the free energy, but that there is no clear argument to get the weight functions. You obtained two series based on two choices, one fitting series (A2) to the high-temperature series to as many terms as known, the other choosing (1,0,0) leading to a different series. The first way you have no result, as you have no more than the known series terms.

The second way can be disproved by series, providing the first few terms of the well-known high-temperature series are rigorously established. The older proofs are correct but not easy to read. Therefore, I gave a much simpler proof with mathematical precision.

My proof does not depend on the papers by Lebowitz and Penrose and by Gallavotti et al., contrary to what you seem to suggest. Also, the statements about these papers are taken out of context:

The statement Re$\beta > 0$ on page 102 in Commun. Math. Phys. 11, 99 (1968) is needed when the gas model has no hard core. Section II opens with the statement that analyticity at $\beta = 0$ can be shown for a hard core potential. The Ising model is equivalent with a lattice gas version with at most one particle per lattice site (empty-occupied becomes spin $+/-1$), a special case of a hard core on the lattice. Thus this objection of yours does not apply.

The statement about $\beta > 0$ in [10] on page 3 of your response arXiv:1209.3247 does not appear explicitly in [10]. It appears near the bottom of the left column of page 494 of Phys. Lett. A 25, 493 (1967). This is a very short letter without much detail. To prove a finite radius of convergence you need to prove an inequality with a positive β. Then $\beta = 0$ will be included within the radius of convergence. Your statement means that the Gallavotti et al. letter was poorly written at that point, [probably due to printer error as Phys. Lett. did not allow authors to correct proofs], not that it is wrong. Also, as said before, I used nothing of these two papers, so that these objections are misplaced.

The next objection that βf does not exist at $T=\infty$ is also invalid. The combination $\beta f=-\ln 2$ there, as f has a simple pole at $\beta=0$. One finds that f has a Laurent expansion with pole term $(-\ln 2)/\beta$ followed by a power series in β with a finite radius of convergence. Statistically, at $\beta=0$ all states have equal probability and there is no phase transition, as not only βf, but also all correlation functions are analytic at $\beta=0$, in spite of the fact that interactions are turned on.

When you expand $\lambda = Z^{1/N}$ in (A12) and (A13) of the original 117 page paper, you expand $\exp(-\beta f)$, which is equivalent to expanding βf. This makes your objection to expanding βf unreasonable. The finite radius of convergence proof that I gave proves that (A13) is not correct.

You bring up that $1/Z$ has a zero at $\beta=0$ in the infinite system. But this is again misleading. Yang–Lee theory is only about the zeroes of partition function Z: When zeros pinch the real temperature axis in the large system limit, then there is a phase transition. There is no theorem for $1/Z$.

This pinching cannot occur, as the proof given by me can be extended to the double expansion of βf in β and βB. The proof for the more general cases is in the old literature. From this joint analyticity at $\beta=0$ and $\beta B=0$, it follows that zeros are a finite (nonzero) distance away, contradicting the pinching that you claim.

Remark 2.4 in my comment and similar statements now make it possible to test your free energy with Monte Carlo methods, as one can now estimate both the systematic error due to finite size and the statistical error due to Monte Carlo methods.

Also, the latest various experimental and theoretical estimates for α are significantly different from 0, see the review of Pelissetto and Vicari, which is [28] in my comment. Please, check the accuracies reported of large numbers of theoretical and experimental works that are discussed there.

Next, the use of dimensionless $K_i=\beta J_i$ and $h=\beta H$ can be done in more than one way. The partition function and correlation functions (and βf) only depend on these combinations. That some authors set $\beta=1$, does not mean a loss of the high-temperature case. If you have the result in the K_i and h, you also can choose a new β, say β', and write in the results $K_i=\beta' J_i$ and $h=\beta' H$. There is no loss of the high-T limit $\beta'=0$. Again this is an objection that is invalid and it does not apply to my latest comment, as I nowhere used $\beta=1$, nor did I use results from authors that did.

Finally, the last paper arXiv:1110.5527 is based on an incorrect solution of the 3D Ising model. There are problems I noted: With ϕ a phase, $|e^{i\phi}|=1$, thus formula (4) contains phases that drop out. Also, having three independent Virasoro algebras means that you have the 3+1 dimensional space rewritten as a 6-dimensional (2+2+2) space, the “product” of three independent 2-dimensional spaces. Things do not add up.

This is my answer to your “Any further criticisms or comments from you are welcome.”